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IGNITION QUALITIES OF HYDROCARBONS IN THE DIESEL-FUEL BOILING RANGE

BY

A. D. PUCKETT AND B. H. CAUDLE

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IGNITION QUALITIES OF HYDROCARBONS IN THE DIESEL-FUEL BOILING RANGE[1/]

By A. D. Puckett[2/] and B. H. Caudle[3/]

This paper summarizes present knowledge of the ignition qualities of pure hydrocarbons likely to be present in modern Diesel engine fuels, as shown by an extensive search of the technical literature. The report also discusses the possible significance of cetane number and hydrocarbon structure. Cetane or cetene numbers, and other physical properties, are tabulated for about 100 hydrocarbons, and a bibliography is appended.

In recent years the Diesel engine has enjoyed increasing popularity due to its dependability, inherent characteristics of fuel economy, and the fact that it operates on a fuel that hitherto has been available in comparatively large quantities at a low price. These qualities have enabled the compression-ignition engine to compete very favorably with other types of prime movers in many fields and have led to predictions of further rapid expansion in the application of Diesel power. In a survey of the field of all petroleum fuels for combustion engines, Holaday et al (9) have predicted that by 1948 railroads will be using 10 times as much Diesel fuel as was used in 1939 and that over-all consumption will have doubled that of 1939. Other estimates of the yearly demand for Diesel fuels five years hence vary from 2.6 to 5 times the amount used in 1944.

Into this picture has come the question of whether the greatly increased production to meet this estimated demand is compatible with the maintenance and possible improvement in quality of fuels necessary to satisfy future engines. Unfortunately perhaps for the Diesel engine, factors other than those of simple arithmetical multiplication must be considered. For example, the consumption of oil in central heating plants doubled from 1935 to 1943, and a further increase of 57 percent of the 1943 demand is expected by 1950. Jet propulsion has been developed to the stage where it is entirely practical for military aircraft. Catalytic cracking plants, many of which were constructed to meet the wartime accelerated demand for high-octane gasoline, are taking their place in the refining industry. All these developments, as well as the Diesel engine, require material of approximately the same boiling range. Virgin gas oils make excellent burner fuels, perform most satisfactorily in the gas-turbine units for aircraft according to present information, and are at a premium as catalytic cracking stock.

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These considerations have led a number of organizations to embark on programs of research aimed at the development of fundamental data upon which to base future improvement in compression ignition fuels and engines and the assembling of information needed if it becomes necessary to augment the supply with synthetic products or to improve the ignition quality of material not now considered desirable. The Bureau of Mines, in informal cooperation with the Western Petroleum Refiners Association, the Coordinating Research Council, and the Society of Automotive Engineers, is one of the organizations engaged in this research. This paper is the first of those projected dealing with Diesel fuels and summarizes present knowledge of the ignition qualities of pure hydrocarbons.

The only widely accepted engine test for the suitability of a fuel for Diesel use is that for ignition quality, usually expressed in terms of cetane number; yet there are available in the literature very few engine data on the cetane numbers of individual hydrocarbons. As was stated late in 1945, "comparatively little research has been done with a view toward developing superior Diesel fuels. Research in this country is at about the level of gasoline research in the 1920's" (8).

Early work of Ricardo in England and of Boerlage and Broeze in Holland revealed that the high-speed Diesel engine was quite sensitive to fuel-ignition quality. In this country in 1933 the Volunteer Group for Compression Ignition Research was organized with a membership of representatives from interested laboratories, both governmental and industrial, to develop a method of rating Diesel fuels. In 1937, at the request of the Compression Ignition Group, the Automotive Diesel Fuels Division of the Cooperative Fuel Research Committee was formed to continue this work; as a result, the CFR committee issued a proposed method of test in 1938 (2), which was adopted as a tentative method by the American Society for Testing Materials in 1941. This method was revised slightly in 1943, and as ASTM Designation D613-43T, "Tentative Method of Test for Ignition Quality of Diesel Fuels", is in use today. By this method, the ASTM cetane number of a Diesel fuel is defined by and is numerically equal to the percentage by volume of normal cetane in a mixture of cetane and alpha-methylnaphthalene which the fuel matches in ignition quality when compared by the prescribed procedure. Thus, by definition, alpha-methylnaphthalene has a cetane number of zero, and normal cetane, of 100. The test engine is a 3¼-inch bore x 4½-inch stroke, continuously-variable-compression, precombustion-chamber-type Diesel and is loaded by a constant-speed electric motor. Conditions under which the engine is operated in making a test are shown in Table 1.

In addition to the ASTM test, there have been a number of other engine-test methods (28); as a result, the hydrocarbons that have been rated in an engine (and they number only approximately 20) were not tested in exactly the same manner. Apparently, however, the various procedures correlate well with one another, and the values appear comparable. There also has been considerable study of the combustion characteristics of Diesel fuels in bombs. Of these investigations, results of the work of

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Michailova and Neumann (13) show good correlation with the engine test and have received wide distribution. These investigators used an apparatus, subsequently referred to as either the Neumann or the Neiman bomb, which consisted of a metal bomb equipped with a fuel-injection system and suitable instrumentation for indicating the time of injection and pressure rise following ignition of the fuel.

TABLE 1. — Engine operating conditions for ASTM cetane number determination

Engine speed, r.p.m.	Constant, 900 ± 9
Injection advance, deg. BTC	13
Injector opening pressure, p.s.i.	1500 ± 50
Injection rate, ml./min.	13.0 ± 0.2
Jacket temperature, °F.	209 to 215 (constant to within ± 1°F.)
Air-inlet temperature, °F.	150 ± 2

The determination of ignition quality consists of injecting 80 mg. of fuel into the heated bomb, containing air at 580°C. and 21 atmospheres pressure, and determining the time lag between injection and combustion. This ignition lag or induction period is then converted to equivalent cetene number by comparison with a calibration curve of cetene number versus ignition lag. This curve is based on engine determinations using as reference fuels cetene with an assigned value of 100 cetene number and alphamethylnaphthalene with an assigned value of 0 cetene number. The cetene scale thus established appears to be linearly related to the cetane scale by the following equation (10): Cetane number = 0.875 x cetene number. The Russian authors list results of tests of eight fuels for which bomb and engine ratings differed by two cetene numbers or less. These few data, however, appear to be the only strictly comparable results in the literature, and further confirmation is needed.

In 1938 Russian scientists, notably A. D. Petrov and coworkers, began a study of the hydrocarbons in the Diesel-fuel boiling range directed toward finding compounds distinguished by low pour points, and ignition qualities in the order of 40 to 50 cetene number. So far, they have synthesized and tested more than 60 hydrocarbons (17), and the results of their work have been made available generally in this country through translations by J. G. Tolpin, which have appeared in the Universal Oil Products Company Survey of Foreign Petroleum Literature. These ignition quality ratings were determined by the Neumann bomb method; but, as Petrov points out, the bomb appears to agree with the engine. That they are expressed in cetene rather than cetane number is unfortunate but does not preclude their comparison with values determined by the ASTM test, as there is evidence indicating a linear relation between the two rating scales (5).

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The Russian data on ignition quality and those of other investigators are shown in Tables 2 through 5, which also include other physical properties of the hydrocarbons. These tables contain all the available information on ignition qualities of pure hydrocarbon compounds determined under conditions which approach Diesel engine operation.

One prime objective of the collection of ignition-quality data should be the application of relationships derived from them to a complete solution of the problem of predicting cetane numbers for the remaining possible hydrocarbons or types of hydrocarbons in the Diesel-fuel boiling range. It is interesting to note that for some time it has been known that normal paraffins have the highest cetane numbers. In 1935 Boerlage and Broeze (3) listed, in approximate order of decreasing ease of ignition in an engine, the following structural types: (a) Paraffin, (b) olefin, (c) benzene nucleus, and (d) condensed ring. In 1941 Ju and Wood (10) reported the order of decreasing cetane number to be: (a) Straight-chain paraffins, (b) naphthenes, and (c) isoparaffins. Commenting on his data, Petrov (17) states, "Considering the enormous number of isomers possible for hydrocarbons with from 10 to 26 carbon atoms, these data furnish only an initial orientation in the problem of the dependence of antiknock properties (cetane numbers) and pour points upon the structure of the fuel hydrocarbons and indicate the outlook for synthetic Diesel fuels only to a slight extent----.

(Apparently in his work Petrov considers "Antiknock" as equivalent to high cetene value, and such statements as "depress antiknock qualities" should be interpreted to mean lower cetene values. As in this country cetane number rather than cetene number is used to express what Petrov appears to call "antiknock quality" the authors have inserted parenthetical interpretations of his statements in terms of cetane numbers.)

"The following are deemed to be the most important conclusions from the data shown: ------.
"1. ---- Isoparaffins of interest for their low pour points and high cetene numbers are those distinguished by a T-like structure. -------- among the paraffins with 12-16 carbon atoms those should be preferred possessing inextensive branching and a single side chain, for introduction of a second side chain depresses sharply their antiknock properties (decreases cetane numbers). Among paraffins with more than 16 carbon atoms, low pour points are inherent only in hydrocarbons with two side chains. In these hydrocarbons the higher molecular weight is responsible for quite satisfactory antiknock properties (acceptable cetane numbers), with exception of symmetrical hydrocarbons, ------. Introduction of a double bond into the molecule of a paraffin decreases the antiknock properties (decreases cetane numbers) considerably less than introduction of a side chain.
"2. ---for a correct evaluation of the quality of Diesel fuels the use of the bomb or a Waukesha engine should definitely be preferred to the formerly widely employed method of evaluation based on determination of the Diesel index.
"3. ----------"

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"4. Monoalkylated benzenes with 12 to 24 carbon atoms, when possessing a branched side chain, show sufficiently low pour points, but satisfactory antiknock properties (acceptable cetane numbers) are observed in them only if they possess more than 16 carbon atoms. -----. When compared to monoalkylbenzenes of the same composition, monoalkylnaphthalenes show much lower antiknock properties (lower cetane numbers). ----------.
"5. Hydrogenation of the benzene ring raises the cetene number by from 9 to 10 points. A higher effect, amounting to 15-20 points or still more, is produced by hydrogenating a naphthalene ring. ----------. Both monoalkylcyclohexanes and monalkyldecalins differ little from aromatics in viscosity, but are characterized ------- by lower pour points and higher cetene numbers; ----------.
"6. As to components of Diesel aviation fuels, this discussion points to the following types of compounds as being of major interest; monoalkylbenzenes with long, but inextensively branched, chains and monoalkyldecalins with short chains--further, mixtures of these hydrocarbons in which the high antiknock properties (high cetane numbers) of one type and the low pour points of the other are made use of. Apparently, of still higher rate of interest will be low solidifying branched paraffins and olefins of the structure types discussed above."

Thus, the work of Petrov and associates has, in general, confirmed the conclusions of other investigators and has extended them considerably. Their observations regarding isoparaffins with T-like structures, alkylbenzenes, alkylcyclohexanes, and alkyldecalins should be of interest if low-pour-point Diesel fuels are ever to be made synthetically. However, the extent of agreement with these conclusions depends upon the point of view. Whereas the Russian program was aimed at finding hydrocarbons having cetene numbers of the order of 40 to 50, many specifications in this country call for 50 cetane number, which corresponds to 57 on the cetene scale. Of all the hydrocarbons listed, less than 30 would meet that requirement.

From the data available, it appears that cetane number bears a linear relationship to the number of carbon atoms in the molecule for normal paraffins, increasing by about 5 units for each additional carbon in the chain between 7 and 16. However, additional ratings on a few of the intermediate homologs would be desirable either to substantiate or disprove this relation. Further work on the effect of varying the position and length of the side chains also seems to be indicated, both for the isoparaffins and the alkylated cyclic compounds. Specifically, it appears that ratings on cyclopentane derivatives, which apparently have been neglected altogether, and on cyclohexanes, might furnish desirable information. Also, extension and confirmation of Petrov's work on alkyl aromatics is desirable. The imperative need for studies on naphthenes and aromatics is indicated by recent calculation by the Bureau of Mines that the average distillate between 400°F. and 700°F. throughout the country contains 55 percent naphthenes, 20 percent aromatics, and only 25 percent paraffins.

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Eighty-seven percent of the distillates in this range contain more than 50 percent naphthenes, and 77 percent contain more than 20 percent aromatics. It is of further importance that this boiling range includes the naphthenic and aromatic dicyclic hydrocarbons (both condensed and conjugated rings) which have low cetane values.

Use of these data would be greatly facilitated if all were in terms of cetane number. That few hydrocarbons have been rated by both the ASTM engine and the Neumann bomb and that in some cases there is disagreement should be recognized. For example, Cloud and Ferenczi (4) report an engine rating of 80 cetane number for normal dodecane, whereas the bomb value obtained by Petrov was 82 cetene number which would be equivalent to 70 on the cetane scale. Further engine work may indicate that a conversion factor can be used with confidence to convert the bomb ratings to ASTM cetane numbers, and in any event, the bomb data indicate trends which should point the way to further research.

Certain general trends of ignition quality with structure have been pointed out, and it is to be hoped that additional information will permit quantitative estimation of cetane numbers from structural formulas. However, there are exceptions to any generalized statements in this regard. For example, normal octyldecalin might be expected to have a higher ignition quality than either propyl decalin or normal octylbenzene. Petrov lists the cetene numbers of these three hydrocarbons as 35, 40, and 36, respectively. Whereas 9-methylheptadecane might possibly be expected to rate higher than tetradecene-1, the reverse is true. Such exceptions emphasize the fallacy of predicting ignition qualities from scanty information.

In conclusion it can be stated, that although many data on ignition qualities of hydrocarbons are available, they are not strictly comparable, and spot checks, at least, of the bomb cetene numbers by the ASTM engine test would be highly desirable. Further extension of the available information, either by rating judiciously selected hydrocarbons by the ASTM method or a bomb using the present reference fuels and calibrated directly against the engine, may furnish a basis for quantitative deduction of cetane number from chemical structure. For work of this nature the bomb, as compared to the ASTM engine, has the undeniable advantage of requiring extremely small samples of the material under test. The Bureau of Mines is currently working on a bomb similar to that originated by Michailova and Neumann, and if this apparatus can be correlated with the ASTM test, it will be used to add to the data on cetane numbers of pure hydrocarbons.

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TABLE 2. - Ignition quality and related properties of paraffin hydrocarbons

		1	2	3	4	5	6	7	8	9	References								
											column								
No.	Hydrocarbon	Empirical formula	Cetane no.	Cetene no.	Boiling point, °C.	Pour pt., °C.	Flash pt., °C.	D_4^{20}	Aniline pt., °C.	n_D^{20}	1	2	3	4	5	6	7	8	9
1	3-Methylpentane	C_6H_{14}	30[a]	-	63.2^{760}	-118.0[b]	-	0.66409	69.3	1.3765	-	-	-	7	7	-	10	6	7
2	n-Heptane	C_7H_{16}	57 56[a] 55	-	98.4^{760}	- 90.5[b]	- 2.0	.68375	70.6	1.38774	-	10	-	7	6	6	7	6	7
3	2,2,4-Trimethylpentane	C_8H_{18}	12[a]	17	99.3^{760}	-107.45[b]	- 9.0	.69194	80.4	1.39157	-	-	10	7	7	6	7	6	7
4	n-Dodecane	$C_{12}H_{26}$	80	82	216.2^{760}	- 12	73.9	.7493	83.7	1.42182	-	4	14	7	14	6	7	6	7
5	3-Ethyldecane	$C_{12}H_{26}$	-	55	$201.5\text{-}2.5^{760}$	- 70	-	.7519[c]	-	1.424	-	-	19	19	19	-	19	-	19
6	4,5-Diethyloctane	$C_{12}H_{26}$	-	23	$192\text{-}4^{760}$	- 70	-	.7632	-	1.4279	-	-	23	6	14	-	6	-	6
7	2,2,4,6,6-Pentamethylheptane	$C_{12}H_{26}$	-	10	176^{737}	- 70	-	.7468	-	1.4191	-	-	14	6	14	-	6	-	6
8	2,5-Dimethylundecane	$C_{13}H_{28}$	-	66	214-6	- 70	-	.7850	-	1.4242	-	-	14	19	19	-	19	-	19
9	4-Propyldecane	$C_{13}H_{28}$	-	45	215^{757}	- 65	-	.7703	-	1.4354	-	-	14	16	14	-	16	-	16
10	5-Butylnonane	$C_{13}H_{28}$	-	61	213^{753}	- 70	-	.7587	-	1.4355	-	-	16	16	16	-	16	-	16
11	2,7-Dimethyl-4,5-diethyloctane	$C_{14}H_{30}$	-	45	117^{13}	- 70	-	.7767	89.5	1.42886	-	-	14	6	14	-	6	6	6
12	n-Hexadecane (cetane)	$C_{16}H_{34}$	100	110	280^{760}	20	110.0	.7749	95.1	1.4352	-	-	14	7	14	6	7	6	7
13	7,8-Dimethyltetradecane	$C_{16}H_{34}$	-	46	$268\text{-}70^{760}$	- 70	-	.7921	-	1.4430	-	-	14	7	14	-	6	-	6
14	7-Butyltridecane	$C_{17}H_{36}$	-	80	147^{12}	- 70	-	.7779	-	1.4355	-	-	16	16	16	-	16	-	16
15	9-Methylheptadecane	$C_{18}H_{38}$	-	75	173^{10}	- 8	-	.7810	-	1.4388	-	-	14	16	14	-	16	-	16
16	8-Propylpentadecane	$C_{18}H_{38}$	-	55	206	- 65	-	.7911	94.8	1.4444	-	-	14	23	14	-	23	14	23
17	7,8-Diethyltetradecane	$C_{18}H_{38}$	-	77	$139\text{-}41^{19}$	- 36	220.0	.7871	93.8	1.4397	-	-	14	6	14	6	6	14	6
18	5,6-Dibutyldecane	$C_{18}H_{38}$	-	34	156-7	- 62	210	.7911	94.8	1.4421	-	-	14	6	14	6	6	14	6
19	9,10-Dimethyloctadecane	$C_{20}H_{42}$	-	68	$138\text{-}52^{2}$	- 55	-	.8147	-	1.452	-	-	14	26	14	-	26	-	26
20	7-Hexylpentadecane	$C_{21}H_{44}$	-	95	$183^{9.5}$	- 61	-	.7909	-	1.4419	-	-	16	16	16	-	16	-	16
21	2,9-Dimethyl-5,6-diisoamyldecane	$C_{22}H_{46}$	-	55	153-5	- 38	-	.7984	101.8	1.4442	-	-	14	6	14	-	6	6	6
22	9,10-Dipropyloctadecane	$C_{24}H_{50}$	-	54	$174\text{-}7^{1\text{-}2}$	- 60	-	.8100	-	$1.454^{18.5}$	-	-	14	26	14	-	26	-	26
23	9-Heptylheptadecane	$C_{24}H_{50}$	-	100	210^{8}	- 27	-	.7995	-	1.4465	-	-	16	16	16	-	16	-	16

a/ Bureau of Mines laboratory determination by ASTM D613-43T.
b/ Freezing point.
c/ D_4^{20} calculated from sp. gr. at different temperature.

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Table 3.- Ignition quality and related properties of olefin hydrocarbons

No.	Hydrocarbon	1 Empirical formula	2 Cetane no.	3 Cetene no.	4 Boiling point, °C.	5 Pour pt., °C.	6 Flash pt., °C.	7 D_4^{20}	8 Aniline pt., °C.	9 n_D^{20}	References column 1	2	3	4	5	6	7	8	9
"A"	Olefins																		
1	1-Tretradecene	$C_{14}H_{28}$	-	90	$124.5\text{-}5.0^{15}$	- 12	-	0.772	59.8	1.4365	-	-	14	7	14	-	7	6	7
2	1-Hexadecene	$C_{16}H_{32}$	88	100	275^{760}	4.0 a/	-	.7835	72.4	1.4417	-	10	-	10	7	-	7	6	7
3	5-Butyl-4-dodecene	$C_{16}H_{32}$	-	52	$265\text{-}7^{760}$	- 62	-	.7855	-	1.4450	-	-	14	7	14	-	7	-	7
4	Tetraisobutylene	$C_{16}H_{32}$	4.5	5	240.2^{728}	-	96.0	.7960	-	1.4490-5	-	10	10	6	-	6	6	-	6
5	7-Butyltridecene	$C_{17}H_{34}$	-	41	-	- 70	-	-	-	-	-	-	17	-	17	-	-	-	-
6	9-Methyl-9-heptadecene	$C_{18}H_{36}$	-	75	-	- 26	-	-	-	-	-	-	14	-	14	-	-	-	-
7	7,10-Dimethyl-8-hexadecene	$C_{18}H_{36}$	-	49	-	- 57	-	-	-	-	-	-	14	-	14	-	-	-	-
8	8-Propyl-8-pentadecene	$C_{18}H_{36}$	-	52	167.8^{8}	- 71	242.0	.7946	83.8	1.4489	-	-	14	6	14	6	6	23	21
9	7-Hexyl-7-pentadecene	$C_{21}H_{42}$	-	54	-	- 70	-	-	-	-	-	-	14	-	14	-	-	-	-
10	10,13-Dimethyl-11-doeicosene	$C_{24}H_{48}$	-	64	-	- 38	-	-	-	-	-	-	14	-	14	-	-	-	-
"B"	Diolefins																		
1	2,6,7-Trimethyl-2,6-tridecadiene	$C_{16}H_{30}$	-	28	$115\text{-}7^{3}$	-	-	.8055 b/	-	1.4547	-	-	18	18	-	-	18	-	18
2	3,12-Diethyl-3,11-tetradecadiene	$C_{18}H_{34}$	-	30	$171.5\text{-}2.0^{6}$	-	-	.8159	-	1.4630	-	-	14	6	-	-	6	-	6

a/ Freezing point.

b/ Sp. gr. 15.7/4.

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TABLE 4. - Ignition quality and related properties of naphthene hydrocarbons

No.	Hydrocarbon	1 Empirical formula	2 Cetane no.	3 Cetene no.	4 Boiling point, °C.	5 Pour pt., °C.	6 Flash pt., °C.	7 D_4^{20}	8 Aniline pt., °C.	9 n_D^{20}	References column 1	2	3	4	5	6	7	8	9
"A"	Cyclohexanes																		
1	Cyclohexane	C_6H_{12}	13.15[a]	-	80.80^{760}	5.86[b]	- 17.2	0.77867	30.4	1.4262	-	12	-	6	6	6	6	6	6
2	Methylcyclohexane	C_7H_{14}	20[a]	-	100.3^{760}	-126.3[b]	- 3.9	.7692	40.3	1.4230	-	-	-	7	6	6	7	6	7
3	Bicyclohexyl	$C_{12}H_{22}$	53[c]	-	238.5^{760}	4.2[b]	99.0	.8865	48.2	1.4796	-	10	6	-	11	6	11	11	7
4	3-Cyclohexylhexane	$C_{12}H_{24}$	-	41	$87\text{-}9^{10}$	- 70	-	.8297[d]	-	1.4570^{19}	-	-	27	27	27	-	27	-	27
5	2-Methyl-3-cyclohexylnonane	$C_{16}H_{32}$	-	64	$115\text{-}20^{15}$	- 50	-	.8350[d]	-	1.4600^{17}	-	-	27	27	27	-	27	-	27
6	1-Methyl-3-dodecylcyclohexane	$C_{19}H_{38}$	-	80	$177\text{-}80^{5}$	- 14	-	.8247	-	1.4590	-	-	14	21	14	-	21	-	21
7	2-Cyclohexyltetradecane	$C_{20}H_{40}$	-	65	$197\text{-}9^{20}$	- 19	-	.8492	-	1.4740	-	-	21	21	21	-	21	-	21
8	2-Methyl-2-cyclohexylpentadecane	$C_{22}H_{44}$	-	51	$195\text{-}8^{10}$	- 50	-	.8413	94.5	1.4667	-	-	14	21	14	-	21	14	21
9	1,2,4-Trimethyl-5-hexadecylcyclohexane	$C_{25}H_{50}$	-	48	$204\text{-}5^{2}$	- 29	-	.8395	-	1.4640	-	-	21	21	21	-	21	-	21
10	5-Cyclohexyleicosane	$C_{26}H_{52}$	-	75	$231\text{-}3^{4}$	- 9	-	.8364	107.0	1.4642	-	-	14	21	14	-	21	6	21
"B"	Decalins																		
1	Decalin[e]	$C_{10}H_{18}$	-	55	185.5^{760}	- 30	57.7	.8699	35.3	1.46968	-	-	14	6	14	6	6	6	6
2	n-Propyldecalin	$C_{13}H_{24}$	-	40	$245\text{-}7^{743}$	- 69	-	.8789	55.2	1.4776	-	-	22	22	22	-	22	22	22
3	n-Butyldecalin	$C_{14}H_{26}$	-	35	$263.5\text{-}4.0^{760}$	- 68	-	.8829	55.5	1.4817	-	-	14	6	14	-	6	14	6
4	sec-Butyldecalin	$C_{14}H_{26}$	-	38.5	$261.5\text{-}3.0^{741}$	- 68	-	.8831	60.1	1.4798	-	-	22	22	22	-	22	22	22
5	tert-Butyldecalin	$C_{14}H_{26}$	-	27	$263\text{-}4^{763}$	- 50	-	.9047	26.5	1.4972	-	-	14	6	14	-	22	6	6
6	n-Octyldecalin	$C_{18}H_{34}$	-	35	$325\text{-}7^{746}$	- 48	-	.9069	16.7	1.5067	-	-	14	6	14	-	6	6	6
7	4-Methyl-4-decalylheptane	$C_{18}H_{34}$	-	24	$138\text{-}9^{-}$	- 33	-	.9199	-	1.5116	-	-	24	24	24	-	24	-	24
8	3-Methyl-3-decalylnonane	$C_{20}H_{38}$	-	21	$173\text{-}6^{6}$	- 31	-	.9273	-	1.5173	-	-	21	21	21	-	21	-	21
9	2-Methyl-2-decalyldecane	$C_{21}H_{40}$	-	42	$156\text{-}8^{-}$	- 34.5	-	.8813	-	1.4822	-	-	24	24	24	-	24	-	24

a/ Bureau of Mines laboratory determination by ASTM D613-43T.
b/ Freezing point.
c/ Tested neat and in blend with same result.
d/ Calculated from sp.gr. at different temperature.
e/ Petrov does not state whether cis or trans form was tested.

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Table 5. - Ignition quality and related properties of aromatic hydrocarbons

No.	Hydrocarbon	1 Empirical formula	2 Cetane no.	3 Cetene no.	4 Boiling point, °C.	5 Pour pt., °C.	6 Flash pt., °C.	7 D_4^{20}	8 Aniline pt., °C.	9 n_D^{20}	References column 1	2	3	4	5	6	7	8	9
"A"	Benzene & Alkylbenzenes																		
1	Benzene	C_6H_6	0[a] -10[b]	-	80.07[760]	5.49[c]	-11.0	0.87866	<-30.0	1.50096	-	12 10	-	7	7	6	7	6	7
2	Toluene	C_7H_8	- 5[a] -21[a]	-	110.65[760]	- 95.0[c]	10.0	.8369	<-30.0	1.49685	-	24 10	-	6	6	6	6	6	6
3	Xylene[d]	C_8H_{10}	-10[a]	-	-	-	-	-	-	-	-	12	-	-	-	-	-	-	-
4	n-Amylbenzene	$C_{11}H_{16}$	8[b] 18[a]	10	204-5[760]	- 78.25[c]	65.5	.8627	<-12	1.4919	-	10 10	11	10	7	6	7	11	7
5	n-Hexylbenzene	$C_{12}H_{18}$	26 32[a]	30	226-7[760]	- 66.8[c]	-	.8602	<-12	1.4890	-	10 10	11	10	7	-	7	11	7
6	m-Diisopropylbenzene	$C_{12}H_{18}$	-12[b] - 3[a]	-	204.0[760]	<- 65[c]	77.0	.8596	Miscible	1.4884	-	10 10	-	10	6	6	11	-	7
7	n-Heptylbenzene	$C_{13}H_{20}$	35 39[a]	40	240-1[760]	-	-	.8595	<-12	1.4884	-	10 10	11	10	-	-	7	11	7
8	n-Octylbenzene	$C_{14}H_{22}$	-	36	255.5-7.5[747]	- 39.5	-	.8550	<- 5	1.4850	-	-	14	25	25	-	6	6	24
9	2-Phenyloctane	$C_{14}H_{22}$	-	37	123-5[20]	- 70	-	.8661	<-17	1.4837	-	-	14	7	14	-	7	6	7
10	n-Nonylbenzene	$C_{15}H_{24}$	50	57	280-1[760]	-	-	.8584	-12.3	1.4863	-	10	11	10	-	-	7	11	7
11	n-Octylxylene	$C_{16}H_{26}$	-	23	-	- 66	-	-	-	-	-	-	14	-	14	-	-	-	-
12	2-Phenylundecane	$C_{17}H_{28}$	-	58	142-6[6]	- 35	-	.860	8.1	1.4929	-	-	14	6	14	-	6	6	6
13	n-Dodecylbenzene	$C_{18}H_{30}$	68	66	172-3[9]	- 7	-	.8568	13.5	1.4844	-	10	14	10	14	-	7	11	7
14	4-Phenyldodecane	$C_{18}H_{30}$	-	78 48	138-41[3]	- 24	-	.8551[e]	-	1.4850	-	-	11 25	25	25	-	7	-	7
15	7-Phenyltridecane	$C_{19}H_{32}$	-	46	183-4[20]	<- 70	-	.8541	59.8	1.4811	-	-	14	7	14	-	1	1	1
16	n-Tetradecylbenzene	$C_{20}H_{34}$	72	82	195-6[9]	8.6	-	.8567	27.1	1.4812	-	10	11	10	21	-	21	11	7
17	2-Phenyltetradecane	$C_{20}H_{34}$	-	56	185-8[7]	- 7	-	.8555	-	1.4820	-	-	21	21	21	-	21	-	21
18	2-Methyl-2-phenylpentadecane	$C_{22}H_{38}$	-	45	193-5[7]	- 45	250	.8611	-	1.4825	-	-	14	21	14	14	21	-	21

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Table 5. - Ignition quality and related properties of aromatic hydrocarbons (cont.)

No.	Hydrocarbon	1 Empirical formula	2 Cetane no.	3 Cetene no.	4 Boiling point, °C.	5 Pour pt., °C.	6 Flash pt., °C.	7 D_4^{20}	8 Aniline pt., °C.	9 n_D^{20}	References column 1	2	3	4	5	6	7	8	9
19	2-Methyl-4-isobutyl-4-phenylundecane	$C_{22}H_{38}$	-	21	179.8 2.5-7	- 50	-	0.8701 e/	-	1.4998 16	-	-	14	20	20	-	20	—	20
20	2-Methyl-2-phenylheptadecane	$C_{24}H_{42}$	-	45	189-92 8-10	- 40	-	.8861 e/	-	1.5100	-	-	14	20	14	-	20	-	20
21	5-Butyl-5-phenyltetradecane	$C_{24}H_{42}$	-	66	182-5 67	- 48	-	.8559	-	1.4846 12	-	-	25	25	25	-	25	-	25
22	1,2,4-Trimethyl-5-hexadecylbenzene	$C_{25}H_{44}$	-	48	222-4 2	- 6	-	.8782	-	1.4977	-	-	14	6	14	-	21	-	21
23	5-Phenyleicosane	$C_{26}H_{48}$	-	45	235-8 5	28	-	.8514	61.4	1.4813	-	-	21	21	14	-	21	6	21
"B"	Alkenylbenzenes																		
1	2-Phenyl-2-undecene	$C_{17}H_{26}$	-	26	142-6 6	- 22	-	.8599	-	1.4298	-	-	14	7	14	-	7	-	7
"C"	Diphenyls																		
1	Diphenyl	$C_{12}H_{10}$	21 a/	-	254.9 760	69.1 c/	106.0	.9712 f/	-	1.614	-	11	-	7	11	6	7	-	7
2	Diphenylmethane	$C_{13}H_{12}$	11 a/	-	263.2 760	24.8 c/	130.0	1.0059	-	1.5768	-	11	-	7	11	6	7	-	7
3	1,2-Diphenylethane	$C_{14}H_{14}$	1 a/	-	284.7 760	53.0 c/	-	.9661 g/	-	1.5704 25	-	11	-	7	11	-	7	-	7
"D"	Naphthalenes																		
1	α -Methylnaphthalene	$C_{11}H_{10}$	0	0	244.8 760	-	101.1	1.0163	-	1.61494	-	-	-	6	-	6	6	-	6
2	α -n-Butylnaphthalene	$C_{14}H_{16}$	-	7	282.5-3.5 760	- 53	-	.9659	0	1.5790	-	-	14	6	14	-	6	14	6
3	β -tert-Butylnaphthalene	$C_{14}H_{16}$	-	4	272-5 745	- 6	-	.9687	0.0	1.5768	-	-	14	6	14	-	6	6	6
4	2-Methyl-2(β)-naphthylhexane	$C_{17}H_{22}$	-	12	139-40 1	- 32	-	.9579	-	1.5685	-	-	14	24	24	-	24	-	24
5	β -n-Octylnaphthalene	$C_{18}H_{24}$	-	20	335-7 750	- 45.5	-	.9366	0	1.5510	-	-	22	22	22	-	22	-	22
6	4-Methyl-4-(β)-naphthylheptane	$C_{18}H_{24}$	-	10	136-8 1	- 28.5	-	.9522	-	1.5620	-	-	14	24	24	-	24	-	24

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Table 5. - Ignition quality and related properties of aromatic hydrocarbons (cont.)

No.	Hydrocarbon	1 Empirical formula	2 Cetane no.	3 Cetene no.	4 Boiling point, °C.	5 Pour pt., °C.	6 Flash pt., °C.	7 D_4^{20}	8 Aniline pt., °C.	9 n_D^{20}	References column 1	2	3	4	5	6	7	8	9
7	3,6-Dimethyl-3-(β)-naphthyloctane	$C_{20}H_{28}$	-	20	179-82^{6}	- 25	-	0.9494	-	1.5545	-	-	14	21	14	-	21	-	21
8	5-Methyl-5-(β)-naphthylnonane	$C_{20}H_{28}$	-	14	160-62^{1}	- 33	-	.9404	-	1.5520	-	-	24	24	24	-	24	-	24
9	2-Methyl-2-(β)-naphthyldecane	$C_{21}H_{30}$	-	20	158-60$^{0.5}$	- 36	-	.9390	-	1.5310	-	-	14	24	24	-	24	-	24
10	3-Ethyl-3-(β)-naphthylnonane	$C_{21}H_{30}$	-	15	-	-	-	-	-	-	-	-	14	-	-	-	-	-	-
"E"	Tetralins																		
1	n-Propyltetralin	$C_{13}H_{18}$	-	9	256-8^{759}	- 68	-	.9395	0	1.5308	-	-	22	22	22	-	22	22	22
2	n-Butyltetralin[h]	$C_{14}H_{20}$	-	20.5	269-70^{750}	- 62	-	.9312	0	1.5258	-	-	22	22	22	-	22	22	22
3	n-Butyltetralin[h]	$C_{14}H_{20}$	-	16	272-3^{750}	- 64	-	.9331	0	1.5271	-	-	22	22	22	-	22	22	22
4	sec-Butyltetralin	$C_{14}H_{20}$	-	7.8	268-70^{759}	- 58	-	.9356	0	1.5255	-	-	22	22	22	-	22	22	22
5	tert-Butyltetralin	$C_{14}H_{20}$	-	19	265-7^{746}	- 49.5	-	.9349	0	1.5292	-	-	14	6	14	-	6	6	6
6	n-Octyltetralin	$C_{18}H_{28}$	-	20.5	324-6^{740}	- 51	-	.9132	10.8	1.5138	-	-	22	22	22	-	22	22	22
7	di-n-Octyltetralin	$C_{26}H_{44}$	-	29	-	-	-	-	-	-	-	-	14	-	-	-	-	-	-

a/ Blending cetane number.

b/ Extrapolated value.

c/ Freezing point.

d/ Not specified which xylene

e/ Calculated from sp. gr. measured under other conditions.

f/ $D\ \frac{100}{4}$

g/ $D\ \frac{50}{4}$

h/ These compounds are apparently two isomers of n-butyltetralin.

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